SHONKA RESEARCH ASSOCIATES, INC.

Calculation Control Sheet

Calculation number: SRA-96-009 REV. 0

Title: Fitting Uranium Release Estimates of the Purge Cascade

Reason for calculation/revision: New calculation

Client: ChemRisk/TDH

Project: Oak Ridge Dose Reconstruction

Project/Task Number: Task 6

Prepared by: Regan E. Burmeister
Regan E. Burmeister (signed original on file) Date: 10/25/96

Independent Technical Review by: Joseph J. Shonka Date: 10/28/96
Joseph J. Shonka (signed original on file)

Quality Assurance Review by: Deborah B. Shonka Date: 10/28/96
Deborah B. Shonka (signed original on file)

☐ This calculation has been voided or superseded by ____________ (calculation number)

#3246

CALC NO SRA-96-009 **REV** 0

Project/Task ChemRisk/TDH Oak Ridge Dose Reconstruction

Prepared by R. E. Burmeister **Date** 10/25/96 **Checked by/Date** JJS / 10/28/96 J. J. Shonka (signed original on file)

Title Fitting Uranium Release Estimates of the Purge Cascade

Review Method Sheet

The undersigned has reviewed this calculation in accordance with the method(s) indicated below.

	1. Computer Aided Calculation
a	Review to determine that the computer program(s) has been validated and documented, is suitable to the problem being analyzed, and that the calculation contains all necessary information for reconstruction at a later date.
b	Review to determine that the input data as specified for program execution is consistent with the design input, correctly defines the problem for the computer algorithm and is sufficiently accurate to produce results within any numerical limitations of the program.
c	Review to verify that the results obtained from the program are correct and within stated assumptions and limitations of the program and are consistent with the input.
d	Review validation documentation for temporary changes to listed, or developmental, or unique single application programs, to assure that the methods used adequately validate the program for the intended application.
e	Review of code input only, since the computer program has sufficient history of use at Shonka Research Associates, Inc. in similar calculations.
f	Review arithmetic necessary to prepare code input data.
g	Other:
	2. Hand Prepared Calculations
a	Detailed review of the original calculations.
b	Review by an alternate, simplified, or approximate method of calculation.
c	Review of a representative sample of repetitive calculations.
d	Review of the calculation against a similar calculation previously performed.
e	Other:
	3. Revisions
a	Editorial changes only
b	Elimination of unapproved input data without altering calculated results.
c	Other:
	4. Other

Reviewer: Joseph J. Shonka Date: 10/28/96

Joseph J. Shonka (signed original on file)

ABSTRACT

This calculation presents the methodology, justification, and results of fitting the purge cascade emission rates of the Oak Ridge Gaseous Diffusion Plant to statistical distributions. The purge cascade emission rates were previously calculated for the sets of years 1953 - 1955, 1961, 1968 - 1969, 1975 - 1976, respectively (SRA-95-002,011,012,013). Each of these sets of years was statistically analyzed to determine a probability distribution that typified the emission data. In general, the analysis yielded a statistical mean for each data set. Each mean and probability distribution was then used in monte carlo simulations to estimate the mass of UF_6 released for the years of operation that data were unavailable or did not exist. Each simulation was run to a 95% certainty level where it became possible to state that it was 95% probable that the release masses lay within calculated bounds as long as an assumption of similar operating condition remained valid. These bounds are reported below.

TABLE OF CONTENTS

1. INTRODUCTION

Task 6 of the Oak Ridge Dose Reconstruction focuses on the evaluation of the quality of historical airborne and waterborne effluent monitoring data and the determination of the potential significance of unmonitored emissions. Uranium played an important role throughout historical operations on the Oak Ridge Reservation (ORR) and is known to have been released to the environment through air and water. The two largest uses of uranium on the Reservation were the enrichment processes of the ^{235}U isotope by electromagnetic separation at the Y-12 facility and gaseous diffusion at the K-25 facility.

Task 6 activities will be directed at establishing revised uranium release estimates with an associated uncertainty over that of the screening analyses conducted during the Dose Reconstruction Feasibility Study. These activities will support refined assessment of the potential magnitude of health hazards from historical uranium exposures based on both the chemical and radiotoxicity of uranium.

This calculation follows up on the work completed in (SRA-95-002,011,012,013). In those calculations, the purge cascade mass release of UF_6 was estimated for the time periods of Jan. 1953 - Dec. 1955, Mar. 1961 - Dec. 1961, Jul. 1968 - Jun. 1969, and Jul. 1975 - Jun. 1976. For each of these time periods, the purge release estimates that were calculated were representative of longer time periods of operation of the purge cascade; respectively, these were 1947 - 1959, 1960 - 1963, 1964 - 1973, and 1974 - 1985. Data to make purge estimates covering these longer time periods was unavailable or did not exist.

Without actual data the next best method to estimate purge releases for these time periods was to statistically analyze the estimated purge cascade mass releases and determine a probability distribution that described the release for a given time period. Knowing the probability distribution, releases could be simulated with monte carlo software that sampled the specified distributions until a desired mean standard error of a total release for a time period had been achieved. The monte carlo software also determined upper and lower bounds on a total release to any desired percent certainty; in this calculation, that certainty was 95%. The monte carlo simulation provided an easy spreadsheet based tool for interpreting the distribution.

The release amounts determined from the process of fitting and sampling the probability distributions were used to fill in the release estimates for the years of operation. Consequently, it cannot be said that a particular year has an exact and definite release mass, but it can be said with high certainty that a year's release lies within upper and lower bounds as long as operating conditions remain reasonably constant during the period.

2. SUMMARY OF RESULTS

The following table concisely reports the probability distribution fitting results and monte carlo simulation results for the purge cascade. The Distribution column names the distribution that best fit the data for indicated time period. The Trapping Eff. column gives the trapping efficiency of the chemical traps on the purge cascade (SRA-95-010). The Annual (g) column gives the mean value in grams of a 12 month period fitted to the indicated distribution. This value became the asserted release mass into the atmosphere for those years that had no data or data was unavailable. The final two columns give the lower and upper release masses in grams at the 95% certainty level; the release amount for a time period is 95% certain to fall within the limits. The mass numbers reported in Table 2.1 already include the trapping efficiency.

Table 2.1 Annual Release Estimates

Time Period	Distribution	Trapping Eff.	Annual (g)	Lower Limit @ 95% (g)	Upper Limit @ 95% (g)
1947 to 1959	Log Normal	0.15	825	378	1666
1960 to 1963	Extreme Value	0.15	296	195	418
1964 to 1973	Extreme Value	0.15	19	16	22
1974 to 1975	Extreme Value	0.15	21	19	25
1976 to 1980	Weibull	0.15	2204	1807	2759
1981 to 1985	Extreme Value	0.15	21	19	25

There are six time periods listed in Table 2.1. It was found that the data in the 1974 to 1985 time frame were from two different groups of data. The purge cascade emissions during 1976 to 1980 were substantially larger than the emissions in the July 1975 to June 1976 that were estimated in the previous work (SRA-95-013). The statistical analysis of the 1976 to 1980 data is shown in Table 2.1. Examination of that time period revealed that only 1979 had no data, and so 1979 was given the indicated release value. Although the 1974 to 1975 and the 1981 to 1985 time periods are listed separately in Table 2.1, they were part of the 1974 to 1985 period exclusive of the 1976 to 1980 period.

3. METHODS

Two primary methods were used to generate the mass corrections. A commercially available software package for statistical analysis was first used to analyze a particular time period's data. This software determined the type of probability distribution that best described that data. A second commercially available software package for forecasting and risk analysis was used to generate a predicted release mass with upper and lower limits that reflected a 95% certainty in the release amount. The input to this software was the distribution type and parameters determined by the statistical analysis software.

The fitting was performed using the "Probability Distribution Plotting" software (PDP) (TEAM). Following examination of the PDP output, the appropriate distribution was selected, and its coefficients were entered into the modeling software, where the risk assessment was made by Crystal Ball (Crystal). Use of PDP was necessary because Crystal Ball did not provide fitting to distributions. A brief description of the software and their use is as follows:

Using PDP, the data was entered and computations were made for each of the following distributions: normal, lognormal, extreme value, log extreme value with both left and right skew, three parameter Weibull, and a gamma-corrected two-parameter Weibull. Both generalized least squares (GLS) and Ferrell's median regression (MRL) models were employed. GLS was the standard of reference, while MRL was useful in identifying non-typical values caused by sampling errors or pathological sources. Graphs were used to review the fit, and the software also printed a summary, for each distribution module, of the standard error of estimate (SE) plus pass or fail results in runs and confidence limit tests. In theory, the smallest SE using GLS should have indicated the best fit and it was confirmed by passing both the runs and confidence limit tests. The best fit was also reviewed to assure that it was consistent with the distribution that might be expected from the process. When two or more SEs were quite close, the MRL was used as a secondary screen. A drastic difference in SE between regression models usually suggested the distorting influence of outliers. We have used the data from other years of operation as an indicator for the appropriate distribution (if adjacent years follow the log-normal distribution, a year with sparse data where Weibull and lognormal fit equally well would be selected as log-normal). A detailed listing gave classically calculated mean and standard deviation, estimated parameters for the chosen regression model, regression equation, SE, and results of runs and confidence limit tests.

The Crystal Ball software was a forecasting and risk analysis tool for the Excel spreadsheet software. Crystal Ball was written in Excel Version 4 macro language and extended the standard spreadsheet capabilities. A spreadsheet has two major limitations for risk analysis: only one spreadsheet value (or cell) can be changed at a time, making it difficult to examine a range of outcomes; and the "What-if" solver is a single point estimate which does not indicate the probability of occurrence. Crystal Ball extended the spreadsheet by allowing a range of values, described by a distribution, to be placed as the value in a cell. Crystal Ball also permitted Monte Carlo Simulation, in which the distribution was sampled from in a random fashion, displaying the results as a forecast which shows the range of possible outcomes, and their probability, for the range of possibilities associated with the assumptions. This permitted rapid and low cost assembly of a risk assessment model. The monte carlo simulation using Crystal Ball provided a simple way to integrate the distribution and get 95 percentile limits.

4. ASSUMPTIONS

The following assumptions were made in this calculation:

- Because the plant capacity or throughput is unavailable or classified, the purge cascade loss data as calculated for the typical periods represents a valid measure of the purge cascade losses for the intervening periods between two study periods.
- The purge cascade data is a small fraction of the total site release; detailed modeling or calculations for the intervening periods is not warranted.
- Similar operating conditions for the fitted time periods were assumed.
- The trapping efficiency of the chemical traps was assumed to be 0.15 for all years of operation. Trapping efficiency was calculated in SRA-95-010 for the 1945-1946 time frame

5. CALCULATION

The stastitical analysis of the purge cascade release estimates from (SRA-95-002,011,012,013) was performed with the Probability Distribution Plotting© (PDP) software package. Monthly uranium release estimates for four time periods 1953 - 1955, 1961, 1968 - 1969, 1975 - 1976 had been calculated in (SRA-95-002,011,012,013). These four time periods were subsets of longer time periods: 1947 - 1959, 1960 - 1963, 1964 - 1973, and 1974 - 1985, respectively. The release data for the time period 1976 - 1980 came from the ORHS-II Master Release List (SRA-96-012). The PDP software took as input the uranium release estimates and performed a series of tests to determine how well a collection of probability distributions described the data.

Figures 5.1 - 5.5 show the probability distributions for the five time periods. The vertical axis is the probability value which is normalized to one, and the horizontal axis is the release in grams. All the distributions have zero grams as their smallest possible mass release. These figures were generated in Crystal Ball from the distribution parameters that were calculated in PDP. Figure 5.1 depicts a log-normal distribution for the 1953 - 1955 purge cascade data. Those data were monthly estimates of the purge release; this figure gives the distribution that best fit the data. The log-normal distribution is descriptive of simple chemical processes such as gaseous diffusion.

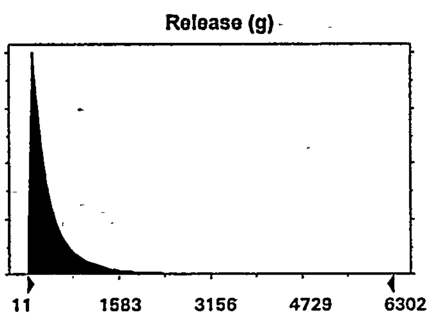

Figure 5.1 1953-1955 Release Distribution

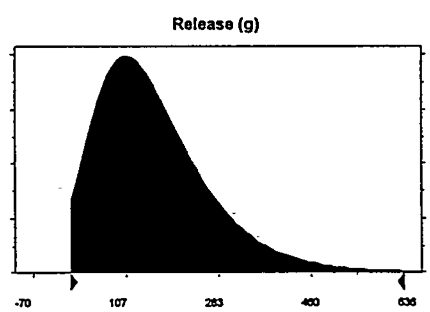

Figure 5.2 1961 Release Distribution

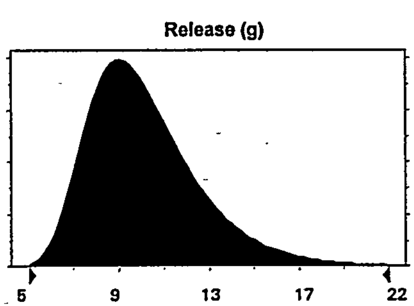

Figure 5.3 1968-1969 Release Distribution

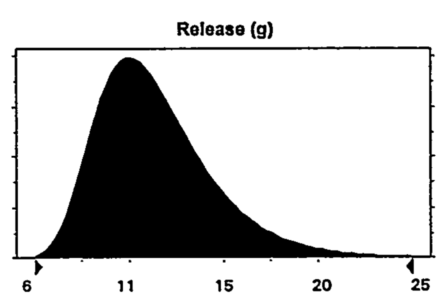

Figure 5.4 1975-1976 Release Distribution

Figures 5.2, 5.3, and 5.4 depict extreme value distributions for the 1961, 1968-1969, and 1975-1976 periods, respectively. Extreme value distributions are descriptive of complex processes involving the combined effects of independent causes each with a different operational form. Figure 5.5 shows a Weibull distribution for the 1976 - 1980 time period. The Weibull distribution is descriptive of processes that involve limits and maxima and minima. It should be noted in the figures that the mass values do not include any reductions due to filter traps.

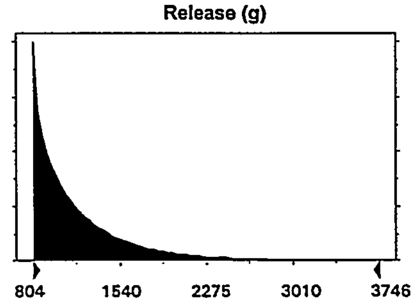

Figure 5.5 1976-1980 Release Distribution

It should be noted that all of the distributions are positively skewed which implied that smaller release values were more probable than large values. The means of these distributions were all larger than the modes, i.e. the most probable values of the distributions, which is another property of positively skewed distributions. One might ask why the same process, the purge cascade, did not have the same distributions over all time periods. Since different amounts were released in each time period, each distribution should have a different mean. The size of each release relative to other releases in each time period determined the probability distribution that best described the data. A variety of processes and plant throughput influenced the amount of purge release, and since these processes and throughput were not constant in time, it is reasonable to expect different distributions to describe the release behavior.

The type of probability distribution and its parameters were given as input to Crystal Ball©, a forecast and risk analysis software package for spreadsheets. For this calculation, the spreadsheet program was Microsoft EXCEL 5.0. In a spreadsheet for a particular time period, a series of 12 cells were named for 12 months of the year and were programmed by Crystal Ball to have a value that was determined by the appropriate probability distribution for that time period. Since the original data were monthly purge amounts, it was necessary to associate each cell with a monthly value determined by the distribution. Another different cell was the sum of the values in the 12 cells; this cell was the total release for a year. The total release cell was programmed by Crystal Ball to be the forecast cell; this cell's statistical behavior was recorded by Crystal Ball and stored for later analysis by the software.

The number of histories or trials to run was set at 30,000. Crystal Ball then ran this many monte carlo samples of the distributions that were programmed for the 12 months cells. Essentially, the 12 month total release was evaluated 30,000 randomly different times, and each month's release was determined from a monte carlo sample of the distribution for that month. It was thought that 30,000 trials would give a sufficiently small mean standard error for each 12 month total.

The following figures are the forecast results from the 12 month totals for the indicated time periods. Each figure names the forecast time period in the title. The left axis gives the probability, and the right axis gives the frequency. The horizontal axis gives the release amounts. In the bottom of each figure is reported the 95% certainty limits. These limits do not include the filter trapping efficiency so they are larger than those reported in Table 2.1. The 95% certainty limits are graphically indicated by the black arrows on the horizontal axis.

Crystal Ball recorded the statistical behavior of the 12 month totals. The mean and mode and other statistical properties were recorded and reported by Crystal Ball. The mean was the average value of the 12 month total; the mode was the most probable value of the 12 month total. The mean standard error was less than 1% for all five 12 month totals. See Tables 5.1 - 5.5 for a full report of the statistics for each 12 month total. It should be noted in the figures that the mass values do not include any reductions due to filter traps.

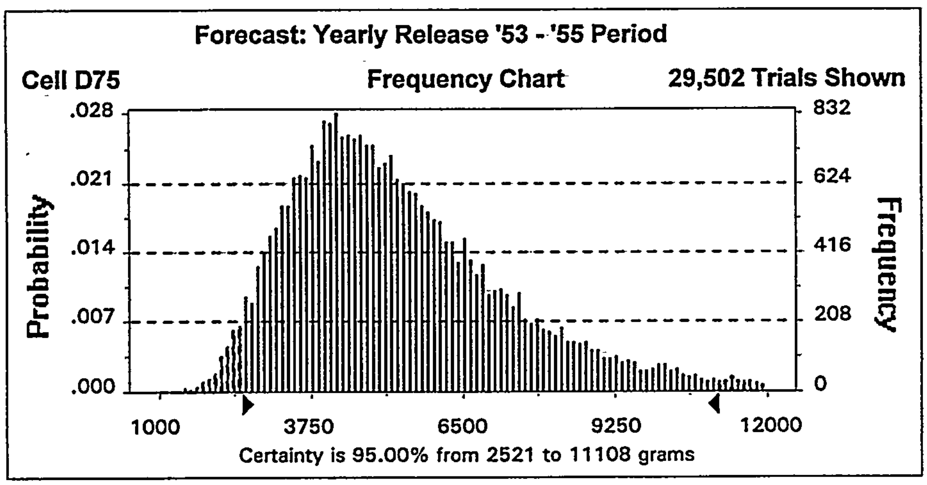

Figure 5.6 Forecast 1953 - 1955

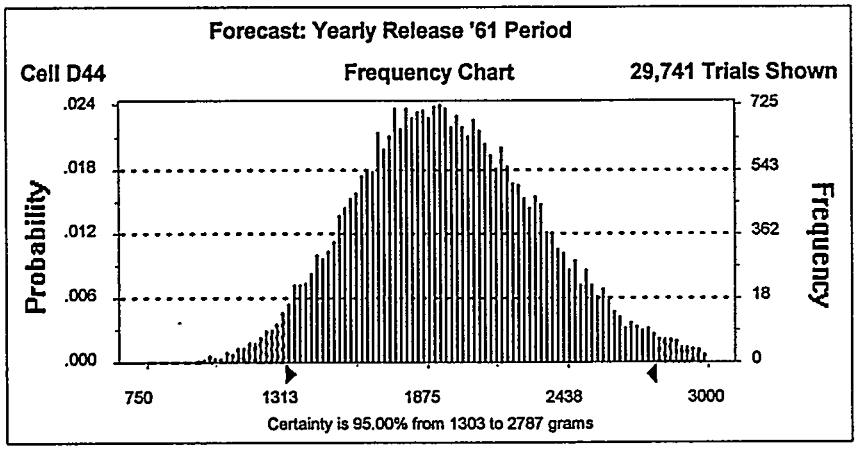

Figure 5.7 Forecast 1961

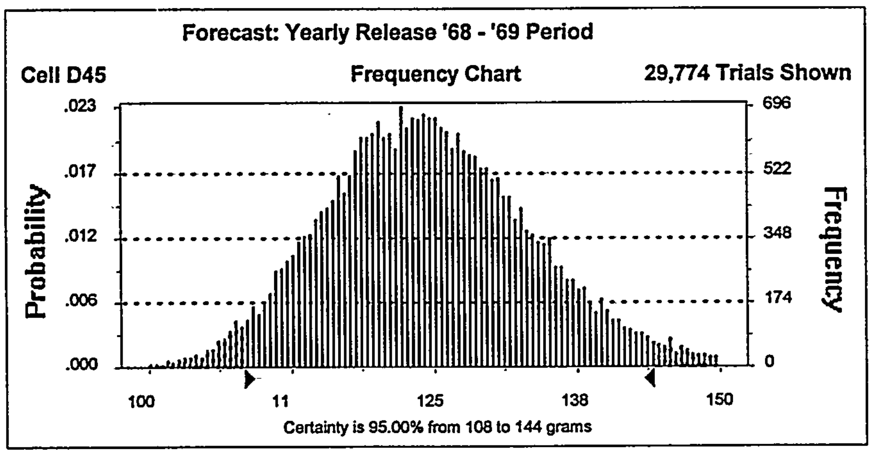

Figure 5.8 Forecast 1968-1969

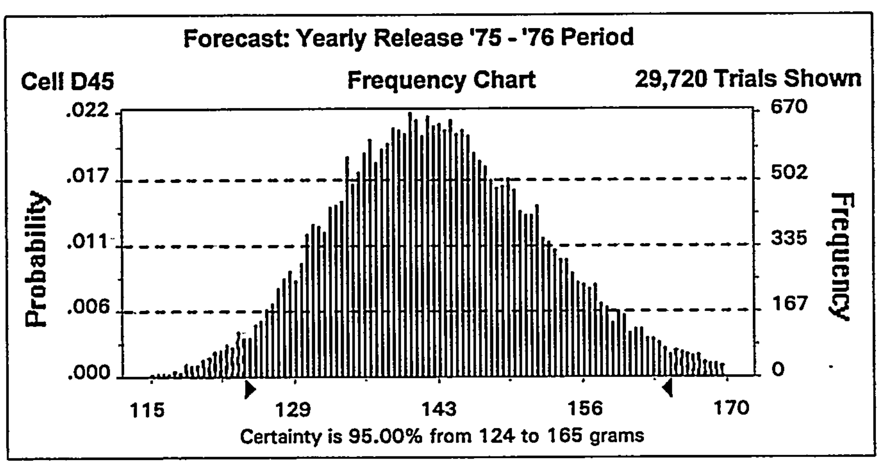

Figure 5.9 Forecast 1975-1976

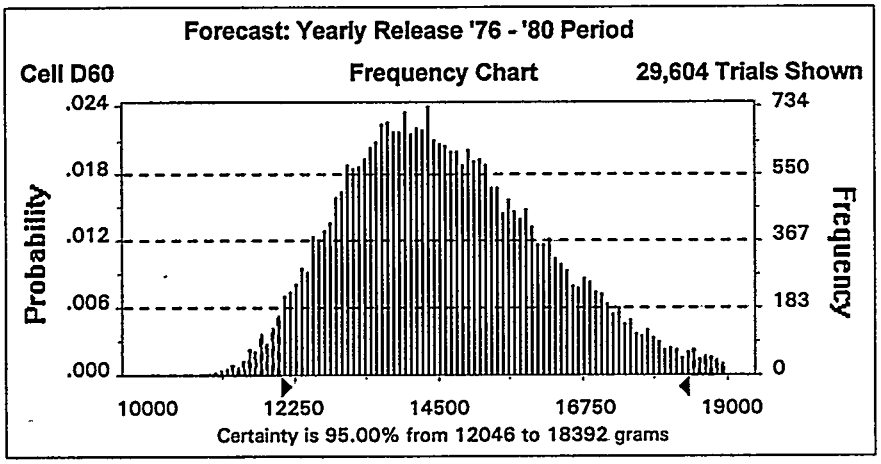

Figure 5.10 Forecast 1976-1980

The following tables were generated by Crystal Ball. They give the statistical report for each of purge cascade time periods. It should be noted that the mass values do not include any reduction due to filter traps. It was only after these numbers had been determined that the trapping efficiencies reported in Table 2.1 were applied to them to give the asserted release values.

Table 5.1 Forecast 1953-1955 Statistics

Forecast: Yearly Release '53 - '55 Period [MAS2.XLS]Cascade Jan 53 - Dec 55 - Cell: D75

Summary:
- Certainty Level is 95.00%
- Certainty Range is from 2521 to 11108 grams
- Display Range is from 1000 to 12000 grams
- Entire Range is from 1311 to 45780 grams
- After 30,000 Trials, the Std. Error of the Mean is 13

Statistics:	Value
Trials	30000
Mean	5498
Median (approx.)	5039
Mode (approx.)	4202
Standard Deviation	2302
Variance	5297440
Skewness	2.15
Kurtosis	15.80
Coeff. of Variability	0.42
Range Minimum	1311
Range Maximum	45780
Range Width	44469
Mean Std. Error	13.29

Table 5.2 Forecast 1961 Statistics

Forecast: Yearly Release '61 Period **[MAS2.XLS]Cascade Mar 61 - Dec 61 - Cell: D44**

Summary:
- Certainty Level is 95.00%
- Certainty Range is from 1303 to 2787 grams
- Display Range is from 750 to 3000 grams
- Entire Range is from 705 to 3907 grams
- After 30,000 Trials, the Std. Error of the Mean is 2

Statistics:	Value
Trials	30000
Mean	1973
Median (approx.)	1949
Mode (approx.)	1874
Standard Deviation	381
Variance	144781
Skewness	0.37
Kurtosis	3.24
Coeff. of Variability	0.19
Range Minimum	705
Range Maximum	3907
Range Width	3202
Mean Std. Error	2.20

Table 5.3 Forecast 1968-1969 Statistics

Forecast: Yearly Release '68 - '69 Period **[MAS2.XLS]Cascade Jul 68 - Jun 69 - Cell: D45**

Summary:

Certainty Level is 95.00%
Certainty Range is from 108 to 144 grams
Display Range is from 100 to 150 grams
Entire Range is from 94 to 169 grams
After 30,000 Trials, the Std. Error of the Mean is 0

Statistics:	Value
Trials	30000
Mean	125
Median (approx.)	124
Mode (approx.)	125
Standard Deviation	9
Variance	84
Skewness	0.34
Kurtosis	3.22
Coeff. of Variability	0.07
Range Minimum	94
Range Maximum	169
Range Width	75
Mean Std. Error	0.05

Table 5.4 Forecast 1975-1976 Statistics

Forecast: Yearly Release '75 - '76 Period **[MAS2.XLS]Cascade Jul 75 - Jun 76 - Cell: D45**

Summary:
- Certainty Level is 95.00%
- Certainty Range is from 124 to 165 grams
- Display Range is from 115 to 170 grams
- Entire Range is from 106 to 188 grams
- After 30,000 Trials, the Std. Error of the Mean is 0

Statistics:	Value
Trials	30000
Mean	143
Median (approx.)	142
Mode (approx.)	141
Standard Deviation	10
Variance	106
Skewness	0.31
Kurtosis	3.13
Coeff. of Variability	0.07
Range Minimum	106
Range Maximum	188
Range Width	82
Mean Std. Error	0.06

Table 5.5 Forecast 1976-1980 Statistics

Forecast: Yearly Release '76 - '80 Period **[MAS2.XLS]Cascade Dec 76 - Feb 80 - Cell: D60**

Summary:
- Certainty Level is 95.00%
- Certainty Range is from 12046 to 18392 grams
- Display Range is from 10000 to 19000 grams
- Entire Range is from 10507 to 23476 grams
- After 30,000 Trials, the Std. Error of the Mean is 9

Statistics:	Value
Trials	30000
Mean	14690
Median (approx.)	14499
Mode (approx.)	14333
Standard Deviation	1634
Variance	2670038
Skewness	0.64
Kurtosis	3.53
Coeff. of Variability	0.11
Range Minimum	10507
Range Maximum	23476
Range Width	12969
Mean Std. Error	9.43

6. REFERENCES

SRA-95-002	Bennett, T.E. Uranium Release Estimates for the ORGDP Purge Cascade 1953-1955. 1995.
SRA-95-011	Bennett, T.E. Uranium Release Estimates for the ORGDP Purge Cascade 1961. 1995.
SRA-95-012	Bennett, T.E. Uranium Release Estimates for the ORGDP Purge Cascade 7/68 - 6/69. 1995.
SRA-95-013	Bennett, T.E. Uranium Release Estimates for the ORGDP Purge Cascade 7/75 - 6/76. 1995.
SRA-95-010	Bennett, T.E. Uranium Release Estimates for the ORGDP Purge Cascade 12/45 - 12/46
TEAM	Probability Distribution Plotting (PDP) Software Version 3.21 for DOS; available from Technical and Engineering Aids for Management (TEAM), Box 25, Tamworth, NH 03866
Crystal	Crystal Ball Version 3.0 from Decisioneering, Inc. 1380 Lawrence Street, Suite 520, Denver, CO 80204-9849
SRA-96-012	Burmeister, R.E. The Master Release List and Source Term for K-25. 1996

7. ELECTRONIC FILES

The following files are included on the diskette that accompanies this calculation.

File Name	Description
SRA009.DOC	This calculation in MS-WORD format
MAS2.XLS	EXCEL spreadsheet of original ESA data for purge cascade for the time periods
MAS2RPT.XLS	EXCEL spreadsheet output from Crystal Ball for monte carlo work

All of the following files are the output from the PDP software. Nomenclature is as follows: CASC1 refers to cascade period 1, the first period in table 2.1; CASC2 refers to the second period, and so on for the other periods. The various extensions to the files are related to all the types of distributions that PDP tests. The *.RAW were the original data files.

CASC1.S2
CASC1.RC
CASC1.R
CASC1.SC
CASC1.S$
CASC1.S1
CASC1.PO1
CASC1.S3
CASC1.S4
CASC1.S5
CASC1.RAW
CASC1.LGA
CASC1.PL1
CASC1.RP1
CASC1.P
CASC1.L
CASC1.PLT
CASC2.P
CASC2.S1
CASC2.R
CASC2.SC
CASC2.S$
CASC2.L
CASC2.S5
CASC2.S2

CASC2.RC
CASC2.S3
CASC2.RPT
CASC2.RAW
CASC2.S4
CASC3.RPT
CASC3.S2
CASC3.RC
CASC3.R
CASC3.S$
CASC3.S4
CASC3.S1
CASC3.P
CASC3.RP1
CASC3.S3
CASC3.RAW
CASC3.L
CASC3.SC
CASC3.S5
CASC4.P
CASC4.L
CASC4.S5
CASC4.S4
CASC4.S2
CASC4.S3
CASC4.R
CASC4.RC
CASC4.RAW
CASC4.S1
CASC4.S$
CASC4.RP1
CASC4.RPT
CASC4.SC
CASC5.S5
CASC5.WEI
CASC5.P
CASC5.LED
CASC5.RC
CASC5.S1
CASC5.RAW
CASC5.S3

CASC5.S4
CASC5.HIS
CASC5.SC
CASC5.S$
CASC5.RPT
CASC5.WEC
CASC5.L
CASC5.S2
CASC5.R